



GroundWater Spatiotemporal Data Analysis Tool (GWSDAT):

Claire Webinar: *Introducing Version 3.1.*



GWSDAT

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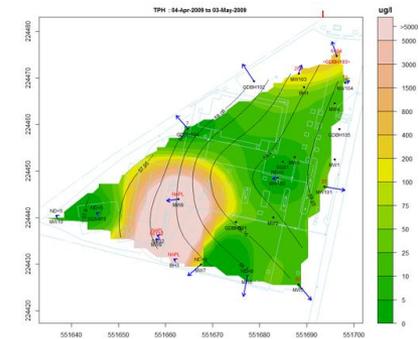
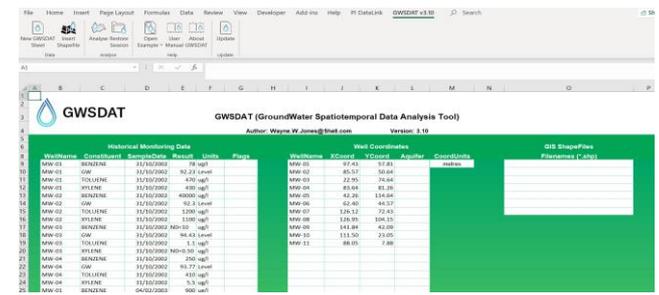
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GWSDAT – what is it?

- User-friendly, open source, **decision support software tool** for analysis & reporting of monitoring data.
- Robust, easy to install, intuitive to use, **requires only standard monitoring data input** (e.g. well coordinates, time series solute concentration data)
- Dataset upload in **variety of formats**, analysis at the click of a button, **export of output** (e.g. PowerPoint), no special expertise or software required.
- Run **locally** on a user's PC / laptop or **online** via web app.
- Works equally well for both **small** (e.g. retail) or **large** (e.g. refinery) sites.



GWSDAT - business benefits

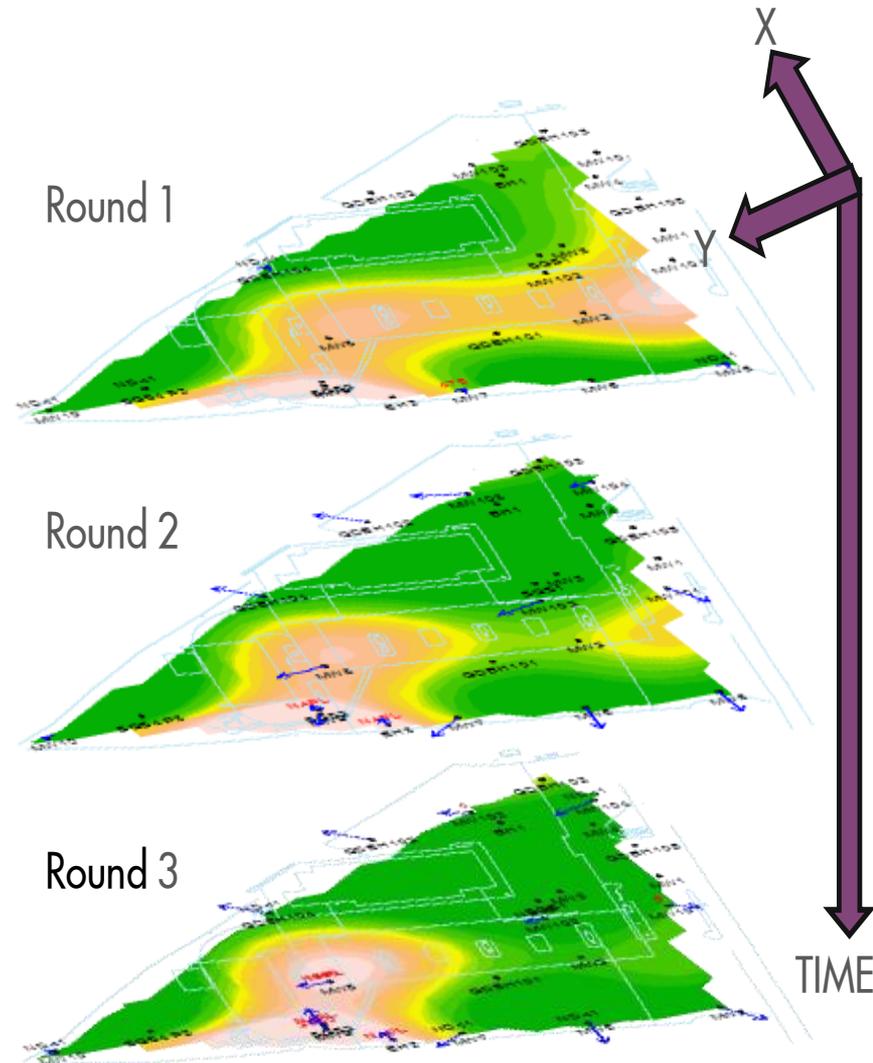
- Tool used operationally in monitoring & assessment of Shell's global downstream assets (e.g. refineries, terminals, fuel stations) for a period of **over 10 years** → achieved **significant efficiencies & savings**, e.g.:
 - Support **design and optimization** of monitoring and/or remediation programs (i.e., avoid collection of redundant data).
 - **Early identification** of potentially new releases, migration pathways, need for corrective action, stable / declining trends that may aid in assessing project closure.
 - **Rapid interpretation** of complex datasets from large monitoring networks (e.g. refineries, terminals).
 - **Efficient evaluation and reporting** of monitoring trends via simple, standardised plots and tables created at the 'click of a mouse'.

GWSDAT – evidence of increased global adoption.

- <http://gwmdat.net/case-studies/> : More than 10 use-cases including Shell, US EPA, Exxon and training videos in Indonesian.
- GWSDAT accepted by regulatory agencies, e.g. adopted as a standard as part of the UK government's guidance for managing contaminated land in England. <https://www.gov.uk/government/publications/land-contamination-risk-management-lcrm/lcrm-stage-1-risk-assessment#GWSDAT>
- GWSDAT LinkedIn user group: <https://www.linkedin.com/groups/8715423/>

GWSDAT trend analysis

- **Smoothing Statistics** to capture the important patterns and trends in the data.
- **Time Series (Temporal) Statistics** to detect trend components.
- **Spatial Statistics:** for modelling geographic relationships.
- **Spatiotemporal Statistics** providing a clear interpretation of contamination plumes



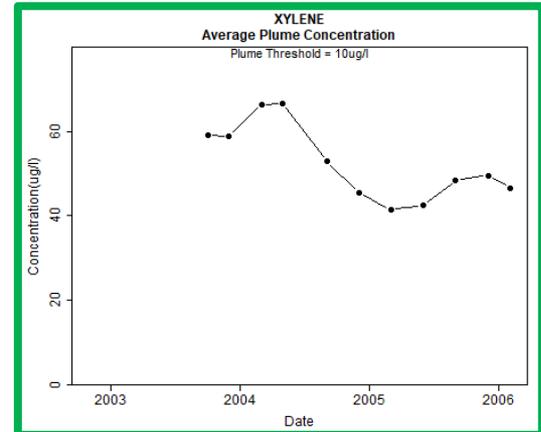
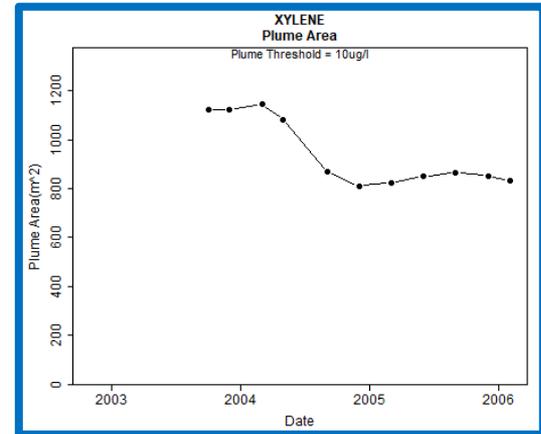
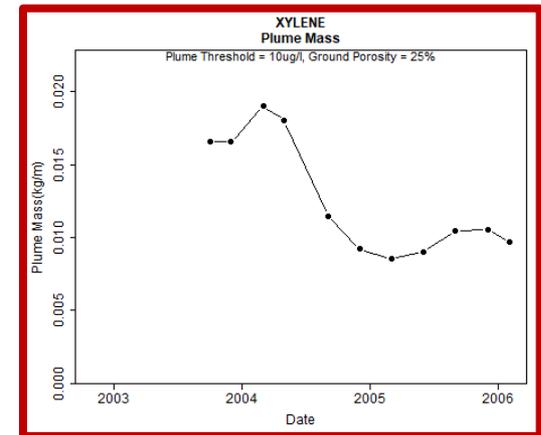
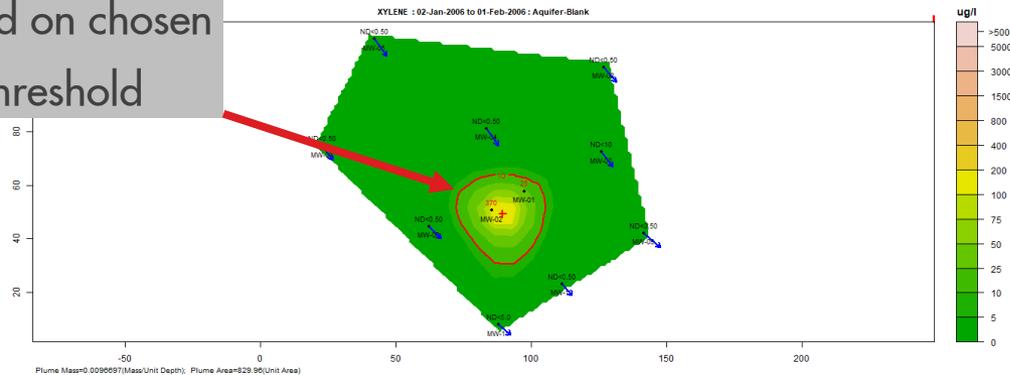
GWSDAT plume diagnostics

■ for a specific analyte:

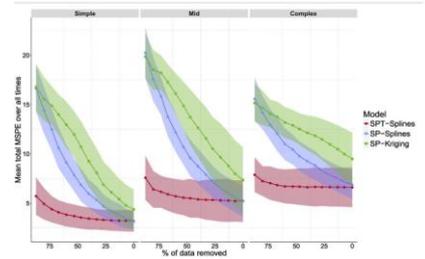
- plume mass
- plume area
- average plume concentration

➔ Evaluation of plume stability

Plume boundary
based on chosen
threshold



Network Optimisation



■ Recent Publication:

“Statistical modelling of groundwater contamination monitoring data: A comparison of spatial and spatiotemporal methods” Science of the Total Environment:

<https://doi.org/10.1016/j.scitotenv.2018.10.231> & PhD Thesis: <http://theses.gla.ac.uk/38975/>

■ Conclusions:

- **More** information using **fewer** observations with a spatiotemporal model
- Spatiotemporal methods can achieve same level of performance but with fewer data points. GWSDAT users are already enjoying this benefit.
- New PhD student started at University of Glasgow, Oct 2021: Implementation of cost-effective spatiotemporal approaches to optimize groundwater monitoring network design and data analysis.
- **Version 3.1** is the beginning of the journey in incorporating **Network Optimisation** tools into GWSDAT.

GWSDAT V3.1 – New Features and Enhancements

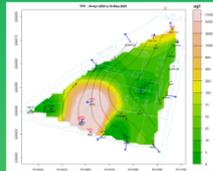
- **Well Redundancy Analysis:** allows user to very conveniently drop a well or a combination of wells from analysis and investigate resultant impact.
- **Updated user manual:** http://gwsdat.net/gwsdat_manual/. Completely overhauled and updated.
- **Excel Add-in:** Updated technology to avoid frequently reported issue of the GWSDAT Excel Add-in menu not being displayed.
- **Updated branding:** Excel data input templates updated with more contemporary colour schemes which align with branding here: www.gwsdat.net.
- **Custom Colour Key:** In response to user feedback added functionality to customise colour key in main GWSDAT spatial plot.
- **Export Contours to ArcGIS:** Export of GWSDAT solute concentrations contours via “tiff” output format.
- **Other minor bug fixes and enhancements.**

GWSDAT V3.1

Demonstration

GWSDAT

An open source, user-friendly, software application for the visualisation and interpretation of groundwater monitoring data.

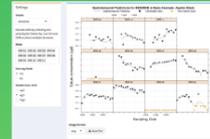


A spatiotemporal model provides a more powerful analysis than spatial modelling at isolated time points or temporal modelling at isolated locations.



Visualisation of site-wide trends in solute concentrations, with interactive control. Trend and threshold matrices can be constructed as summary indicators.

Ease of data entry through a MS Excel spreadsheet containing well co-ordinates and solute concentrations at specific times. Wells can be grouped into separate aquifers. Site maps can be added as GIS shapefiles.



Automatic report generation tools, including site reports and spatial plots at user specified times with groundwater and NAPL data overlaid. Plots can be exported directly to MS PowerPoint.

The simplest form of access to GWSDAT is through the on-line tool.

[GWSDAT on-line](#)

Guidance on use of the tool is available in the [Getting Started](#) page.

A version of the tool which can be installed locally is available either as an [R package](#) from CRAN or as an Excel interface from the [API](#) and [Claire](#).



GWSDAT

GroundWater Spatiotemporal Data Analysis Tool

GWSDAT V3.1 - Updated Add-in menu and branding.

The screenshot displays the Microsoft Excel interface with the GWSDAT v3.10 add-in menu. The menu is located under the 'Add-ins' tab and includes the following options:

- Data:** New GWSDAT Sheet, Insert Shapefile
- Analyse:** Analyse Restore Session
- Help:** Open Example, User Manual, About GWSDAT, Update

The spreadsheet shows the following data:

Historical Monitoring Data							Well Coordinates				GIS ShapeFiles
WellName	Constituent	SampleDate	Result	Units	Flags	WellName	XCoord	YCoord	Aquifer	CoordUnits	FileNames (*.shp)
MW-01	BENZENE	31/10/2002	78	ug/l		MW-01	97.43	57.81		metres	
MW-01	GW	31/10/2002	92.23	Level		MW-02	85.57	50.64			
MW-01	TOLUENE	31/10/2002	470	ug/l		MW-03	22.95	74.64			
MW-01	XYLENE	31/10/2002	430	ug/l		MW-04	83.64	81.26			
MW-02	BENZENE	31/10/2002	40000	ug/l		MW-05	42.26	114.64			
MW-02	GW	31/10/2002	92.3	Level		MW-06	62.40	44.57			
MW-02	TOLUENE	31/10/2002	1200	ug/l		MW-07	126.12	72.43			
MW-02	XYLENE	31/10/2002	1100	ug/l		MW-08	126.95	104.15			
MW-03	BENZENE	31/10/2002	ND<10	ug/l		MW-09	141.84	42.09			
MW-03	GW	31/10/2002	94.43	Level		MW-10	111.50	23.05			
MW-03	TOLUENE	31/10/2002	1.1	ug/l		MW-11	88.05	7.88			
MW-03	XYLENE	31/10/2002	ND<0.50	ug/l							
MW-04	BENZENE	31/10/2002	250	ug/l							
MW-04	GW	31/10/2002	93.77	Level							
MW-04	TOLUENE	31/10/2002	410	ug/l							
MW-04	XYLENE	31/10/2002	5.5	ug/l							
MW-01	BENZENE	04/02/2003	900	ug/l							
MW-01	TOLUENE	04/02/2003	72	ug/l							
MW-01	XYLENE	04/02/2003	7.6	ug/l							

GWSDAT V3.1 – Screenshot - Data Management Page (online version)

GWSDAT Beta

This is a temporary session. [LOG IN](#) [SIGN UP](#)

Data Manager

[Restore Examples](#) [Load Data](#) [Add New Data](#) [Import .csv Data](#) [Import Excel File](#)

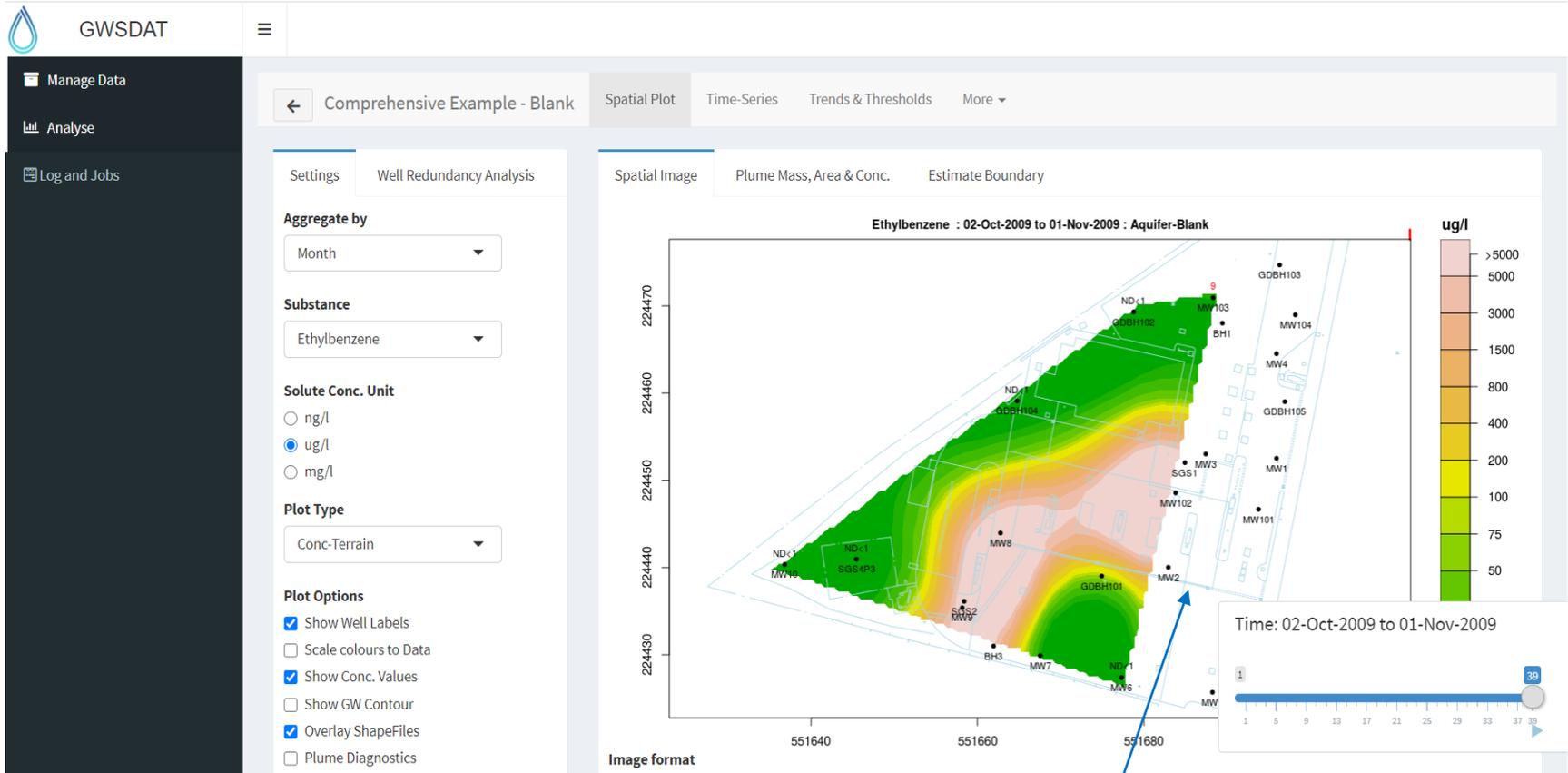
Basic Example -

Contaminants: BENZENE, TOLUENE, XYLENE
Wells: MW-01, MW-02, MW-03, MW-04, ... (11)
Aquifer: Blank

Comprehensive Example -

Contaminants: Nitrate, Sulphate, Ethylbenzene, Toluene, ... (5)
Wells: SGS3P1, SGS3P2, SGS3P3, SGS4P1, ... (6)
Aquifer: Blank, A

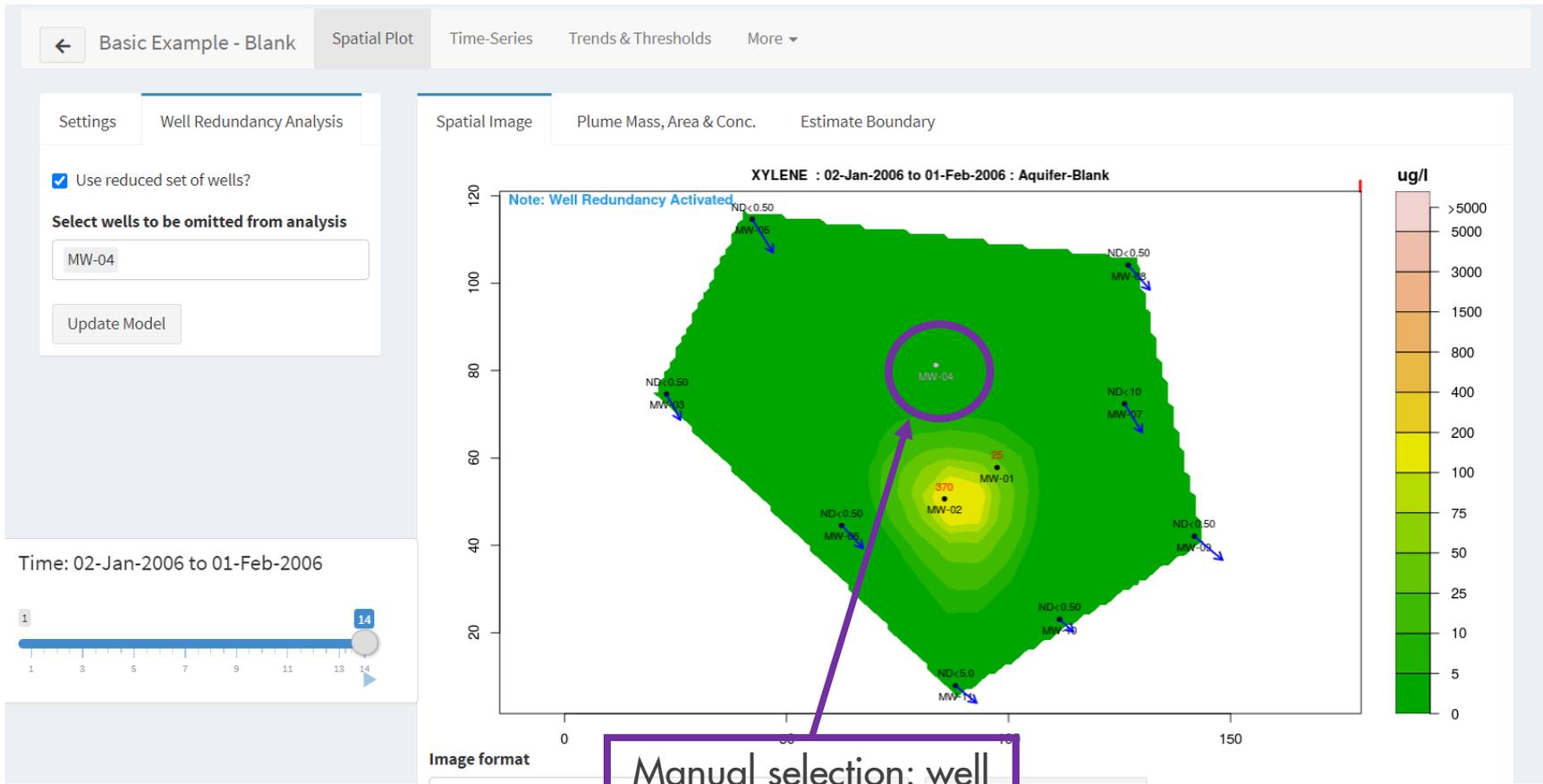
GWSDAT V3.1 – Screenshot - Spatial Plot



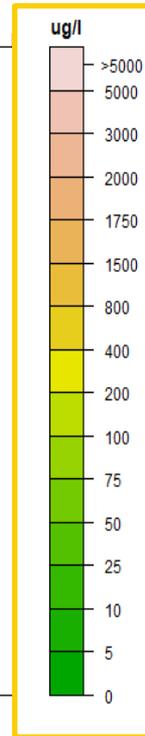
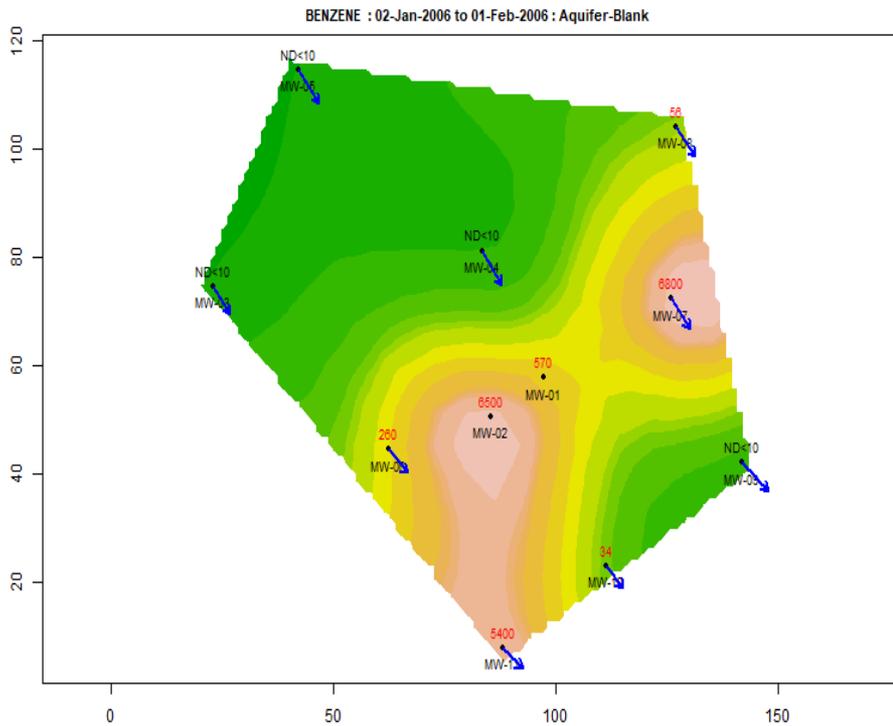
➤ Option to add map of site infrastructure

Well Redundancy – Spatial Image

(Toggle between full model and model with well MW-04 removed)



Ability to customise Spatial plot Colour Key.



Customise the Spatial Plot Colour Key

Specify the contouring intervals for each solute in ug/l.

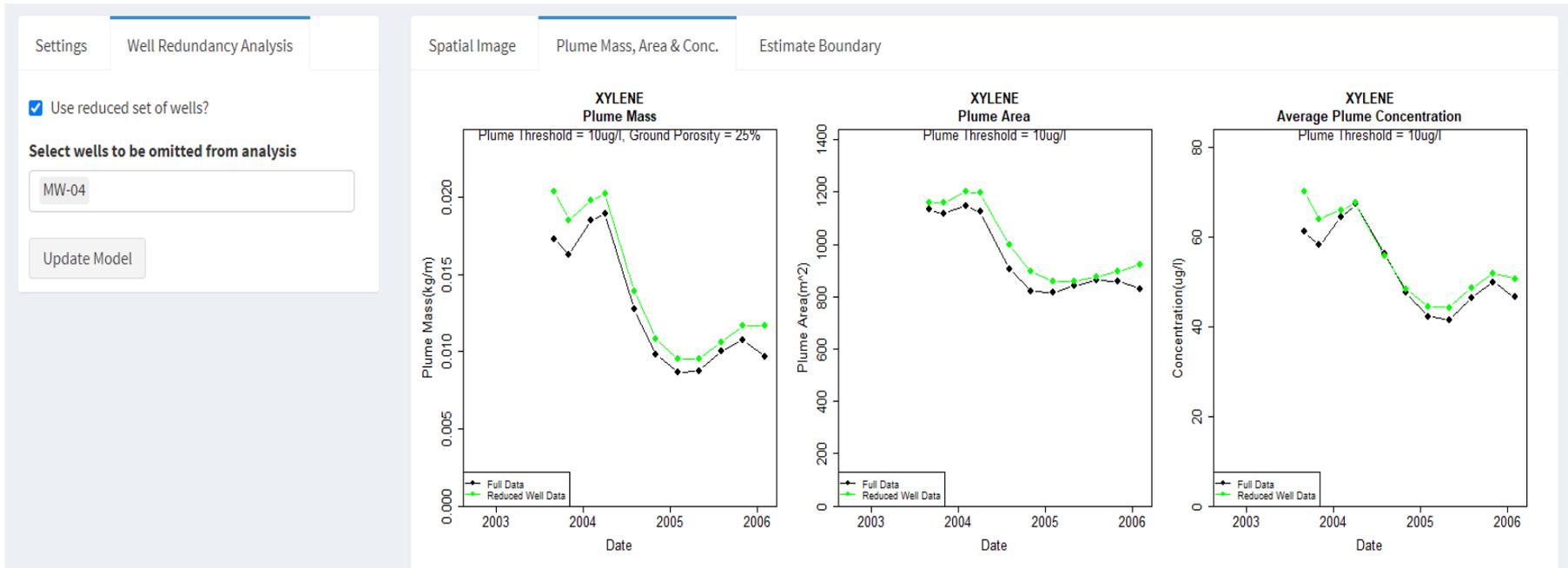
BENZENE	TOLUENE	XYLENE
0.00	0.00	0.00
5.00	5.00	5.00
10.00	10.00	10.00
25.00	25.00	25.00
50.00	50.00	50.00
75.00	75.00	75.00
100.00	100.00	100.00
200.00	200.00	200.00
400.00	400.00	400.00
800.00	800.00	800.00
1500.00	1500.00	1500.00
1750.00		
2000.00		
3000.00	3000.00	3000.00
5000.00	5000.00	5000.00

(Double-click on cells to edit)

(Right-click on cells to add or delete rows)

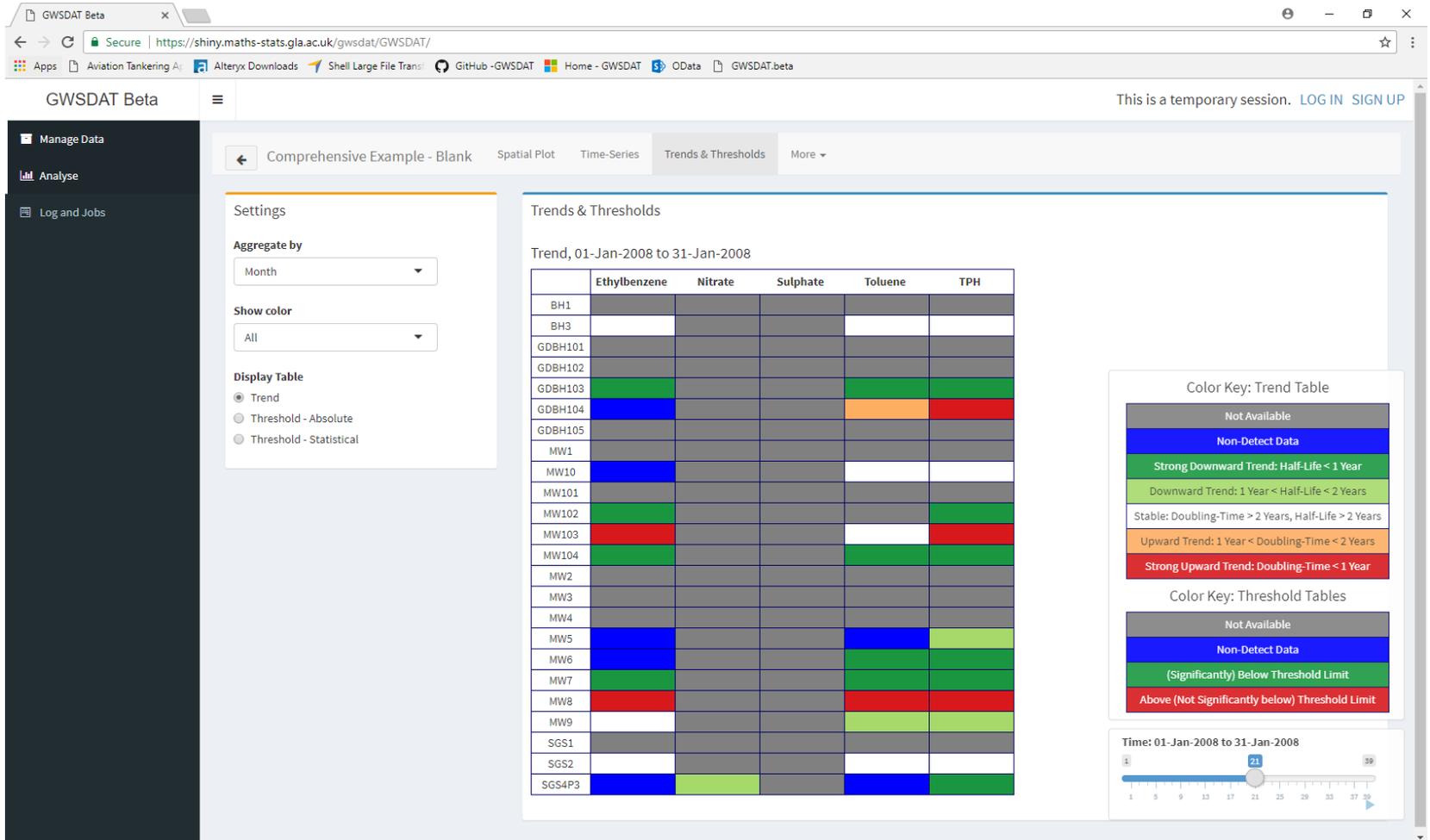
Well Redundancy

(Comparing Plume metrics with well MW-04 removed)

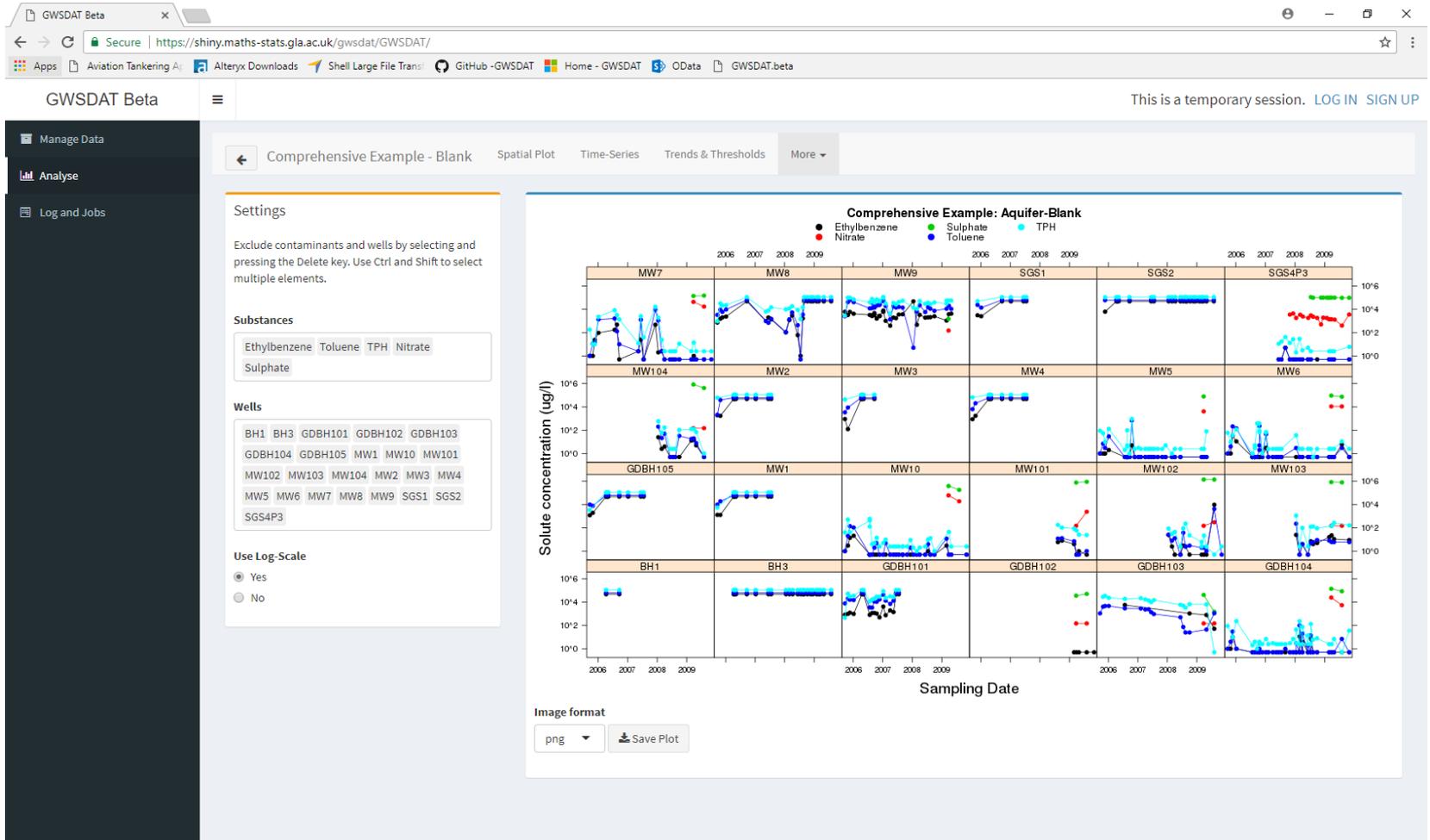


- Black line: original dataset
- Green line: reduced dataset

GWSDAT V3.1 – Screenshot - Traffic Light Plot

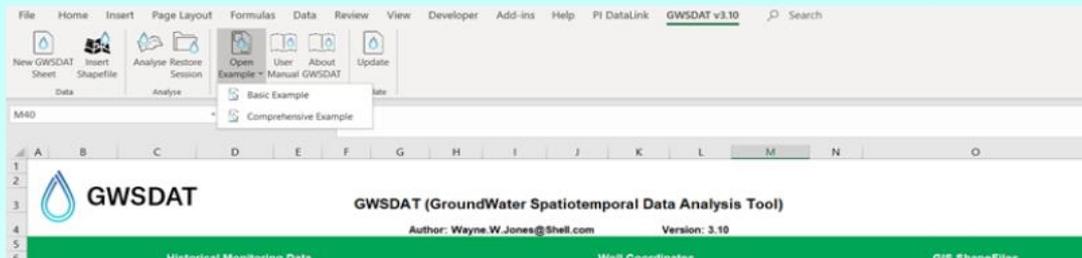


GWSDAT V3.1 – Screenshot - Well Time Series Reporting



GWSDAT Version 3.1 now released!

by Peter Radvanyi | Jun 14, 2021 | Updates



- GWSDAT V3.1 released in August.
- Available to download from: www.api.org/GWSDAT , www.claire.co.uk/GWSDAT and www.gwsdat.net.
- On a longer term basis, we are interested to hear ideas about features related to Well Network Optimisation, e.g. New well placement, Well sampling schemes/strategies, etc.

GWSDAT - Case study: "Service station in New York State"

Case Study: “Service station in New York State”

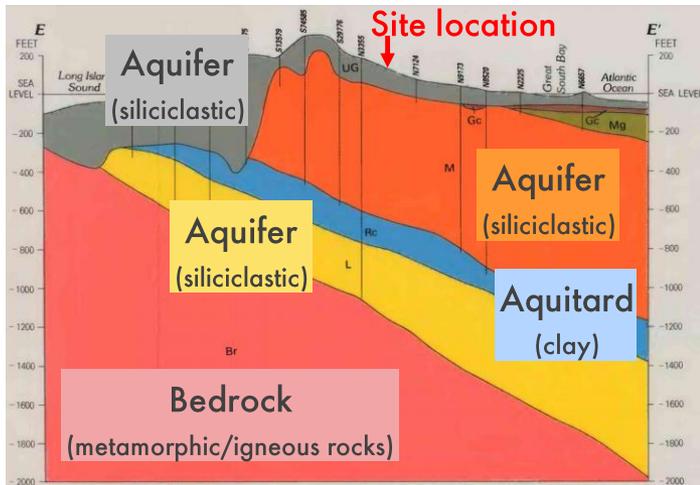
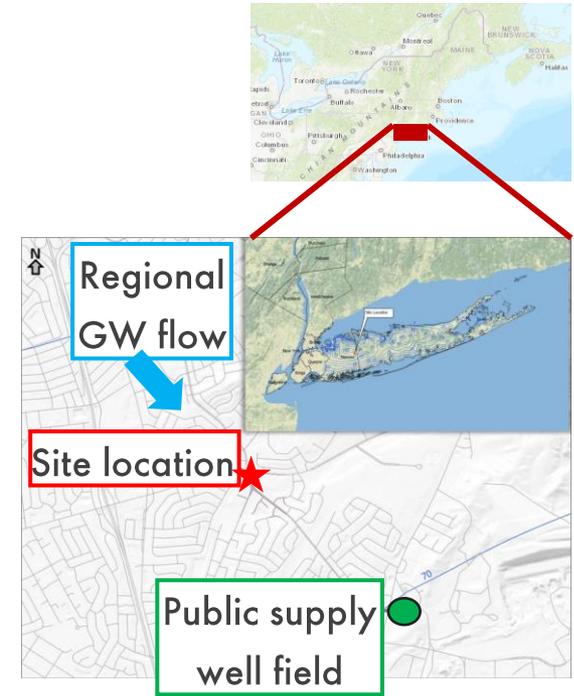
- NYSDEC: agency tasked with protecting public health & environment
- Division of Environmental Remediation:
 - investigation &, if necessary, remediation of impacted sites (e.g. by BTEX)
 - Spatial extent and overall behavior of GW contamination
- GWSDAT is used by NYSDEC staff



For detailed information on case study, please refer to: <http://gwmdat.net/new-york-state/>

Background

- Former service stations located in Plainview, Nassau County, Long Island, New York (USA).
- Historical releases of gasoline → SGW contamination
- GW impact in sole-source aquifer for ~ 1.3 million residents



Wells pre 2019:

* Upper Glacial & Magothy (M) aquifers

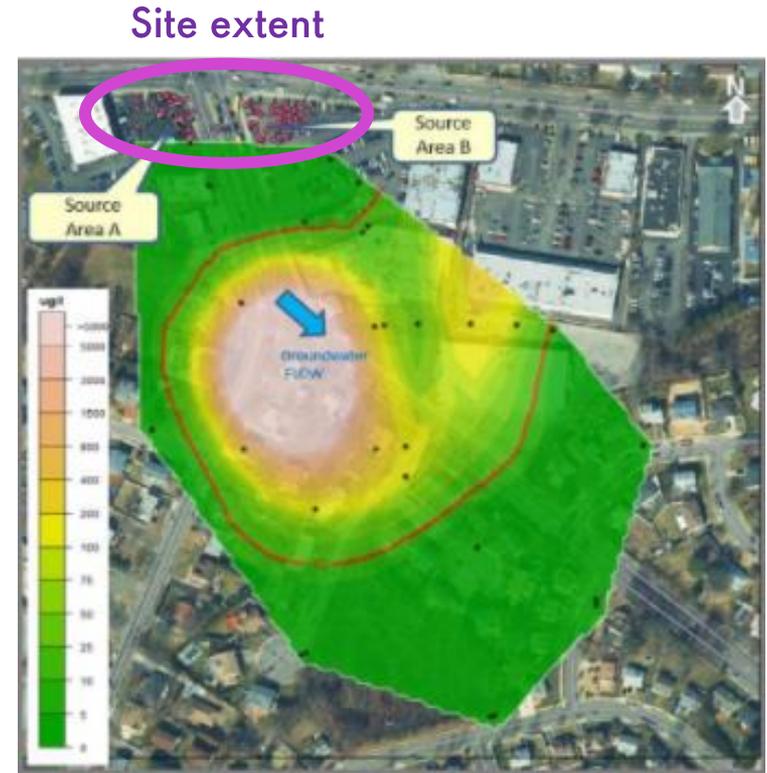
Wells 2019:

* additional deeper wells in M aquifer



Site observation

- Off-site migration of BTEX & MTBE groundwater plume beyond remediated source areas
- Feasibility assessment → final remediation approach: natural attenuation processes
- Questions remaining due to potential impact of public supply well in future



Uncertainties

- Was the off-site benzene plume **adequately delineated** vertically and laterally based on all available data?
- Where is the **potential centreline** of the off-site plume based on the data so that future monitoring wells could be installed at the leading edge and along the centreline of the BTEX plume?
- Was the benzene **plume off-site**, as defined at present time, **stable and/or shrinking**?

- To address some of the above and decide on future project direction
NYSDEC utilized:



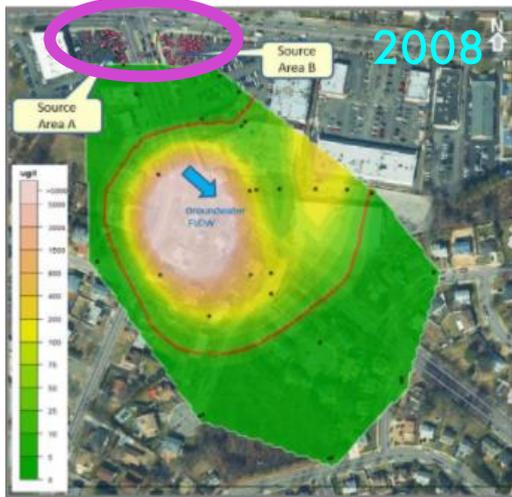
GWSDAT

GWSDAT findings

- Off-site benzene plume was not adequately defined laterally and vertically
- Deeper wells needed to SE → 2019 monitoring campaign confirmed presence of deeper benzene plume

Modeled Benzene plume extent: > 125 ft bgl

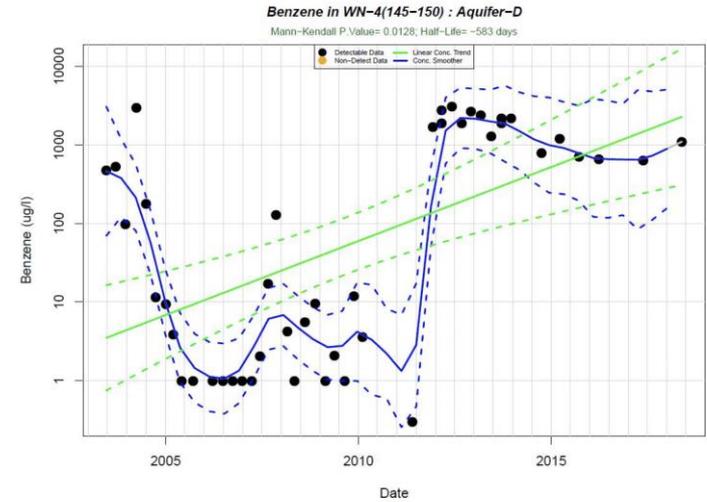
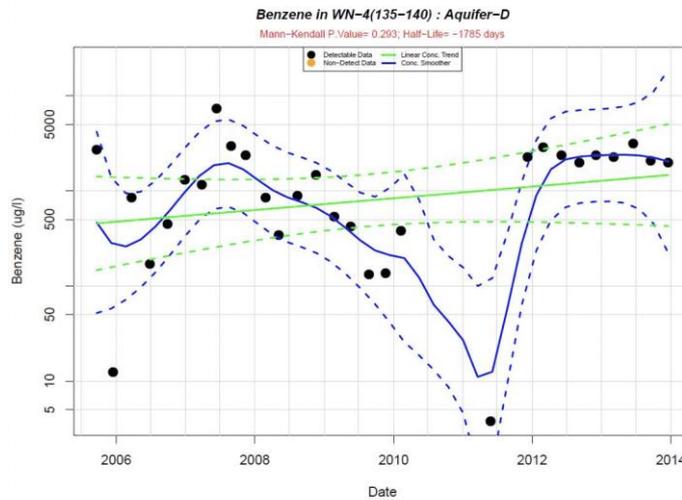
Site extent



GWSDAT findings

- Benzene concentrations **not decreasing** with statistical confidence in deepest monitored portion of aquifer

Benzene plume
stability
assessment
based on
deepest set of
monitoring
wells
(pre 2019)



Synopsis

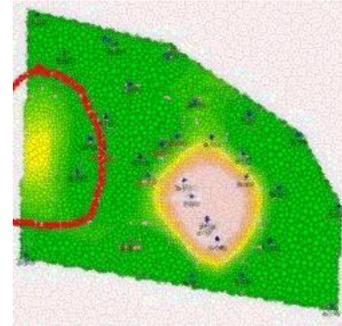
- GWSDAT utilized to address topics such as:
 - residual nature & fate of BTEX plume
 - identified need for more data
 - provided guidance on further site investigation activities
- Outcome:
 - Fewer wells required to be installed
 - GWSDAT to support future decision-making on remediation work (natural attenuation versus more pro-active remediation efforts) → implement most sustainable risk-based remediation method at site

Things to consider..

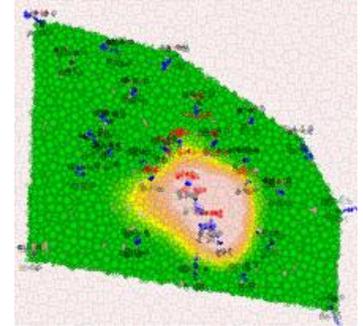
Ballooning..

- Ballooning is a statistical anomaly where predictions can be high in areas where there are no data.

Modelling resolution:
Default & Higher Resolution



Modelling resolution:
10



Nb: data from actual site, figures anonymized

- The best way to improve the model is to up the model resolution...

- See Evers, et al. , 2015. Efficient and automatic methods for flexible regression on spatiotemporal data, with applications to groundwater monitoring, Environmetrics.

References (open access articles)

- Molinari, D. A., 2014. Spatiotemporal modelling of groundwater contaminants, PhD Thesis (Glasgow).
- Jones, et al., 2014. A software tool for the spatiotemporal analysis and reporting of groundwater monitoring data. Environmental Modelling & Software.
- Evers, et al. , 2015. Efficient and automatic methods for flexible regression on spatiotemporal data, with applications to groundwater monitoring, Environmetrics.
- Jones, et al., 2015. Analyzing Groundwater Quality Data and Contamination Plumes with GWSDAT, Groundwater.
- Mclean, M. I., 2018. Spatiotemporal models for the analysis and optimisation of groundwater quality monitoring networks, PhD Thesis (Glasgow).
- Mclean et al., 2018 . Statistical modelling of groundwater contamination monitoring data: A comparison of spatial and spatiotemporal methods. Science of the Total Environment.
- User Manual: http://gwmdat.net/gwmdat_manual/

Q & A

Q&A

Soil and groundwater in Shell

- Contaminated land/groundwater risk assessment and remediation (**corrective**)
- Proactive SGW risk management (**preventative**)
- Project work with consultants (field work, site assessments, remediation)
- Research & development with academia and Joint Industry Projects
- Extensive track record of open publications of scientific work

